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HIGHER-ORDER DIFFERENCING FOR PHASE-FRONT PROPAGATION IN GEOTHERMAL SYSTEMS

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ABSTRACT

We are testing higher-order differencing total variation diminishing schemes implemented in the reservoir simulator TOUGH2 to reduce numerical dispersion of phase fronts in geothermal flow problems. The schemes are called total variation diminishing because they employ flux limiters to prevent spurious oscillations that sometimes occur with other higher-order differencing schemes near sharp fronts. Thus it appears that total variation diminishing schemes rely on an implicit assumption that the overall variability of advected quantities stays constant or diminishes with time. We use the Leonard total variation diminishing scheme in two special problems designed to test the applicability of the scheme for cases where this implicit assumption is violated. In the first problem, we investigate the isothermal propagation of a phase front in a composite porous medium where phase saturation increases as the front enters the second medium. In the second problem, we investigate the propagation of a phase front where boiling increases the saturation difference across the front as it propagates. In the composite porous medium problem, we find that spurious phase saturations can arise if the weighting scheme is based on relative permeability; for weighting based on phase saturation, no such oscillation arises. In the boiling front propagation problem, the front position is highly sensitive to weighting scheme, and the Leonard total variation diminishing scheme is more accurate than upstream weighting because it decreases numerical dispersion in the thermal energy equation.

INTRODUCTION

Strong advective flow of two-phase fluids through fractures occurs during fluid production and reinjection in geothermal systems. The numerical simulation of the propagation of phase fronts by finite difference methods in strongly advective flow systems is affected by numerical dispersion, especially when full upstream weighting is used, a scheme which tends to artificially smooth sharp fronts. Numerical dispersion can be diminished by decreasing grid size, but this can

greatly increase execution times. Another approach for reducing numerical dispersion is to use higher-order differencing schemes.

In higher-order differencing schemes, two upstream gridblocks are used to approximate quantities such as phase saturation (or relative permeability), species concentration, and temperature at interfaces between gridblocks. This is in contrast to upstream weighting which uses only one upstream gridblock. In strongly advective problems and depending on the weighting scheme used, higher-order differencing can result in oscillatory and non-physical values near sharp fronts. These well-known problems have led to the development of total variation diminishing (TVD) higher-order schemes (e.g., Sweby, 1984). TVD refers to the overall variation of quantities in the system tending to diminish with time rather than increase. Thus TVD schemes appear to be based on the assumption that the intrinsic variability of quantities being advected diminishes with time.

While component mass fractions can increase with time by a variety of processes that are independent of flow (e.g., radioactive decay and production [Oldenburg and Pruess, 1996]), some flow processes lead to total variation increasing situations. In this paper, we investigate by numerical experiments using TOUGH2 (Pruess, 1987; Pruess, 1991) two special cases that can arise in geothermal systems where saturation variations increase across a moving phase front with time: (1) a composite porous medium phase propagation problem, and (2) a boiling front propagation problem.

MATHEMATICAL DEVELOPMENT

The accurate approximation of interface quantities is essential for diminishing numerical dispersion in finite difference methods. Below, we briefly review the development of higher-order differencing schemes for the propagation of phase fronts. The development refers to the three gridblocks shown in Fig. 1 where the flow is from left to right as shown by the large arrow. We use fully implicit time-stepping with all quantities taken at the most recent iterative step.

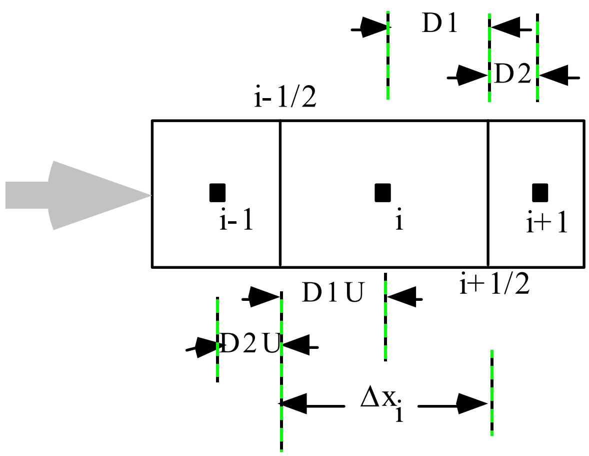

Fig. 1. Three non-uniform grid blocks with flow from left to right. The standard TOUGH2 connection is between i and i+1 and has connection distances $D1$ and $D2$ and an interface at i+1/2. Higher-order schemes use the upstream grid block i-1 with connection distances $D1U$ and $D2U$ and the interface i-1/2.

The phase flux across the interface at i+1/2 is a function of the relative permeability which is a function of phase saturation. Thus at the outset, we are faced with a choice of using a weighting scheme based on either relative permeability (k_r) or phase saturation (S). For upstream weighting or for the case where k_r is a linear function of S, it is immaterial which quantity is used for weighting. However, for typical non-linear relative permeability functions, we will show later that results depend strongly on whether k_r or S is used as the basis of the weighting scheme. For the sake of the development below, we will apply the weighting scheme to S. However, it should be kept in mind that all of the development below can be written in terms of k_r and identical results obtained for many flow problems.

We begin by writing an approximation for S at the $i+1/2$ interface as

$$S_{i+1/2} \approx S_i + D1\left(\frac{S_{i+1} - S_i}{D1 + D2}\right) \qquad (1)$$

which can be rearranged to

$$S_{i+1/2} \approx S_i + \frac{D1}{D1 + D2}\left(S_{i+1} - S_i\right) \quad (2).$$

Defining r, the ratio of upstream to downstream gradients, as follows,

$$r \equiv \frac{\left(\frac{\partial S}{\partial x}\right)_{i-1/2}}{\left(\frac{\partial S}{\partial x}\right)_{i+1/2}} = \left(\frac{\frac{S_i - S_{i-1}}{D1U + D2U}}{\frac{S_{i+1} - S_i}{D1 + D2}}\right) \qquad (3)$$

and rearranging to

$$r \equiv \frac{D1 + D2}{D1U + D2U}\left(\frac{S_i - S_{i-1}}{S_{i+1} - S_i}\right) \qquad (4),$$

we can propose that

$$S_{i+1/2} \approx S_i + \frac{D1}{D1 + D2}\,\phi(r)\left(S_{i+1} - S_i\right) \qquad (5).$$

Depending on the function $\Phi(r)$, different approximations for the interface saturation $S_{i+1/2}$ can be made (see Table 1). For example, if $\Phi(r) = 0$, interface saturation is upstream weighted. If $\Phi(r) = 1$, a weighted average scheme results. For the interface weighting scheme to be TVD, $\Phi(r)$ must fall on the heavy lines or within the shaded regions show in Fig. 2 (e.g., Sweby, 1984; Datta-Gupta *et al.*, 1991; Blunt and Rubin, 1992).

Table 1. Higher-order differencing schemes.

$\Phi(r)$	interface approximation
0	full upstream weighting
1	weighted average
r	two-point upstream
$\frac{(r+\lvert r\rvert)}{(1+r)}$	Van Leer scheme
$2/3 + r/3$	Leonard scheme

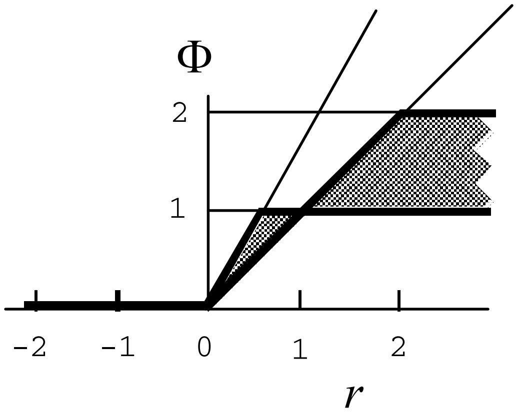

Fig. 2. The heavy lines and shaded regions show the stable values of $\Phi(r)$.

Briefly, the flux limiter is applied to ensure a decrease in the total variation (TV), a quantity defined as

$$TV(S)^{n+1} = \sum_i \left| S_{i+1}^{n+1} - S_i^{n+1} \right| \qquad (6)$$

where n denotes the time level and the sum runs over all gridblocks i. Thus, as Eq. 6 shows, for a typical front propagation problem, the total variation will increase whenever there are jumps or oscillations in the advected quantity, S. We emphasize again that all of the development above can just as well be written for relative permeability, k_r, and correct equivalent weighting schemes derived for many flow situations.

Phase fronts moving with negligible capillary effects self-sharpen due to the effects of relative permeability. This effect tends to reduce numerical dispersion due to upstream weighting, resulting in limited benefits from more accurate higher-order TVD schemes relative to upstream weighting (Taggert and Pinczewski, 1987). Thus, for simple phase displacement processes in uniform porous media, upstream weighting is accurate and efficient. However, there are many cases of phase front propagation in geothermal systems that are complicated by heterogeneity and non-isothermal effects that may benefit from higher-order differencing schemes. This study is directed toward two such cases where the total variation in phase saturation increases with time.

We implemented higher-order differencing schemes in TOUGH2 (Pruess, 1987; Pruess, 1991) with the restriction that the grids used must be either one or two-dimensional with rectangular gridblocks. Within a TOUGH2 simulation, using higher-order TVD schemes entails finding the upstream gridblock, assuming locally one-dimensional flow, calculating $\Phi(r)$, applying the limiters to ensure $\Phi(r)$ is in a stable region of Fig. 2, and approximating interface values of phase saturation, relative permeability, concentration, or temperature accordingly. Verification of the methods implemented into TOUGH2 was presented in Oldenburg and Pruess (1997). The Leonard scheme (LTVD) where $\Phi(r) = 2/3 + r/3$ subject to the limiters shown in Fig. 2 has proven robust and accurate (Leonard, 1984; Datta-Gupta *et al.*, 1991; Oldenburg and Pruess, 1997) and we will explore its use further in the remainder of this paper.

COMPOSITE POROUS MEDIA

In order to investigate the effects of total variation increasing flows, we investigate first the case of phase saturation increasing with flow into a zone of differing relative permeability. This is essentially a Buckley-Leverett problem for a composite porous medium. Analytical solutions for this class of problem were presented by Wu *et al.*, 1993. The case chosen has water injection into a partially saturated composite medium consisting of a fractured rock on the left and a non-fractured rock on the right. The system is isothermal with parameters as given in Table 2 and boundary conditions as shown in Fig. 3.

Table 2. Parameters for composite medium Buckeley-Leverett problem.

Composite porous medium	
Overall length	1 m
Pressure on the left (P1)	103000 Pa
Pressure on the right (P2)	100000 Pa
Liquid saturation on the left	0.5
Liquid saturation on the right	0.21
Initial pressure	100000 Pa
Initial liquid saturation	0.21
Temperature	25 ˚C
Rock 1 (fractured)	
length	0.4 m
Porosity (ϕ)	0.01
Permeability	1 x 10^{-12} m^2
Capillary pressure	0.0 Pa
Relative permeability liquid:	
van Genuchten $\lambda = 0.50$	
$S_{lr} = 0.01$	
$S_{ls} = 1.0$	
Relative permeability gas:	
Corey $S_{gr} = 0.05$	
Rock 2 (unfractured)	
length	0.6 m
Porosity (ϕ)	0.25
Permeability	1 x 10^{-13} m^2
Capillary pressure	0.0 Pa

Relative permeability liquid:
van Genuchten $\lambda = 0.35$
$S_{lr} = 0.10$
$S_{ls} = 1.0$
Relative permeability gas:
Corey $S_{gr} = 0.20$

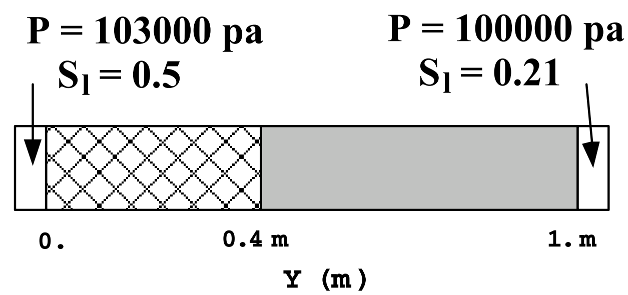

Fig. 3. Schematic of the Buckley-Leverett composite porous medium.

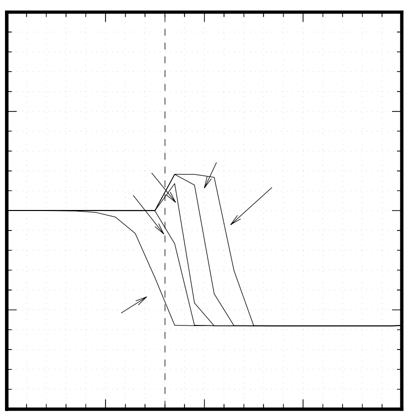

Fig. 4. Liquid saturation for the composite medium Buckeley-Leverett problem with upstream weighting.

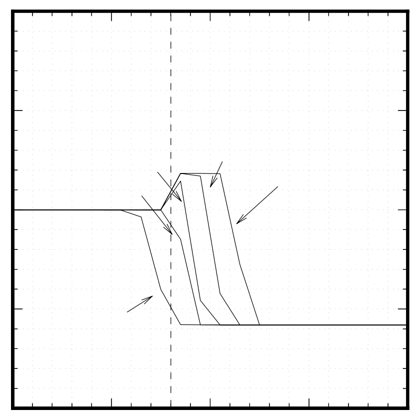

Fig. 5. Liquid saturation for the composite medium Buckeley-Leverett problem with LTVD based on *S*.

Shown in Fig. 4 are results for the saturation front at several different times for the case of upstream weighting. We observe significant numerical dispersion with upstream weighting and the coarse grid consisting of 20 gridblocks in the Y-direction.

Figs. 5 and 6 show the liquid saturation and relative permeability results for the LTVD scheme applied to *S*. In this case, phase saturation is weighted according to Eq. 5 and the corresponding k_r is calculated at the interface. The results show that in this case the phase saturation front is sharper than it is for upstream weighting and saturations are held to physically plausible values. In the LTVD scheme, the phase saturation increases as the front encounters Rock 2, and upstream weighting will be applied locally since the ratio of gradients becomes negative (See Fig. 2 and Table 1). Thus the results in Fig. 5 show that LTVD based on *S* produces sharp phase fronts without spurious overshoots in composite medium problems. Fig. 6 simply shows the corresponding relative permeability for the composite medium. Note in Fig. 6 that k_r is total variation diminishing while *S* is not.

Shown in Figs. 7 and 8 are results for the LTVD scheme applied to k_r at the same times. The LTVD scheme based on k_r also reduces numerical dispersion relative to upstream weighting (c.f., Fig. 4) but note that it has also produced an undesirable overshoot in liquid saturation near the interface between the two porous media.

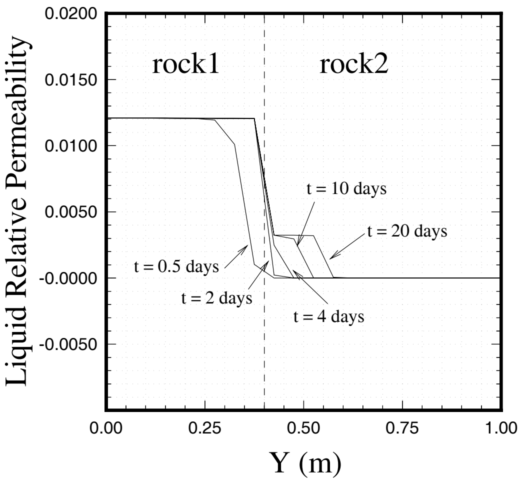

Fig. 6. Relative permeability for the composite medium Buckeley-Leverett problem with LTVD based on *S*.

We present in Fig. 8 the liquid relative permeability (k_{rl}) at the same times. Note that although the liquid saturation is total variation increasing, the relative permeability is total variation diminishing. Thus the LTVD scheme based on k_r has ensured that k_r diminished, but it allowed the undesired effect of the variation in saturation increasing beyond its physical bounds.

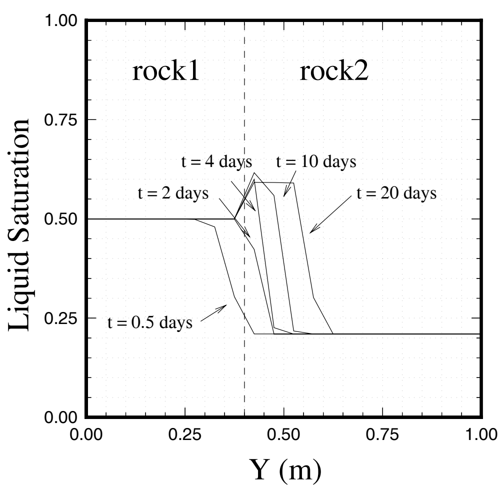

Fig. 7. Liquid saturation for the composite medium Buckeley-Leverett problem with LTVD scheme based on k_{rl}.

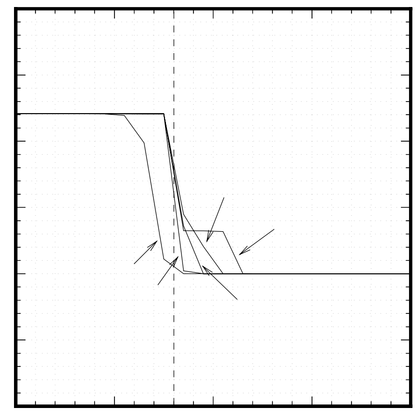

Fig. 8. Relative permeability for the composite medium Buckeley-Leverett problem with LTVD based on k_{rl}.

The differences in behavior when TVD is applied to relative permeability as compared to phase saturation can be understood from the spatial variability of *S* and k_r. While relative permeability varies monotonically near the boundary between the two media, saturation varies non-monotonically (Figs. 5 and 6). Therefore, the ratio *r* of upstream to downstream gradients is always positive for k_r, but is negative for *S* near the boundary. This results in considerably different values for the flux limiter function $\phi(r)$ in this case. In most flow problems, the gradients of *S* and k_r will have the same sign everywhere, so that differences between applying TVD-weighting to *S* or k_r will be minor. However, in problems where saturation and relative permeability gradients differ in sign, as may occur for immiscible displacement in composite media, TVD-weighting may generate significantly different results depending upon whether it is applied to *S* or k_r. As shown above, results are better when the TVD weighting is applied to the advected quantity *S*, rather than the derived quantity k_r. When upstream weighting is applied to interface quantities, as is common practice for problems with propagating phase fronts, there is no difference between applying upstream weighting to saturation or to relative permeability. In the reservoir engineering literature, upstream weighting is usually thought of as being applied to relative permeabilities, or fluid mobilities (Aziz and Settari, 1979; Thomas, 1982). The results obtained here suggest that it would be more appropriate to always think of the interface weighting scheme as being applied to the advected quantity (saturation), as opposed to the derived quantity (relative permeability).

BOILING FRONT

In this problem, cold (T = 30˚C) water is injected into a 200 m long one-dimensional domain. The system is initially nearly single-phase liquid at the saturated vapor pressure (P_0 = 85.93 bar) at T_0 = 300 ˚C. A schematic of the system and initial and boundary conditions is shown in Fig. 9. Parameters for the problem are presented in Table 3.

The evolution begins by injecting cold water at the left-hand side at a rate of 0.4 kg/s and producing mass at the same rate from the right-hand side. The production at the right-hand side lowers the pressure and induces boiling while the cold injection water tends to produce single-phase liquid conditions. The boiling at the right-hand side causes the liquid saturations to decline from the initial conditions. Thus the difference in liquid phase saturation across the moving front increases with time. A two-dimensional version of this problem was presented by Oldenburg and Pruess (1997) with emphasis on the propagation of a tracer front in the liquid phase for a two-dimensional fracture. Here we have further idealized the problem to show the performance of the LTVD scheme in a very simple system and with emphasis on the phase front propagation.

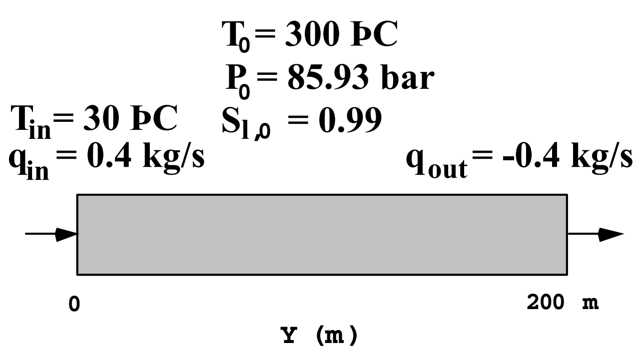

Fig. 9. Boundary and initial conditions for the one-dimensional injection and production problem.

Results for upstream weighting and LTVD differencing schemes with 100 gridblocks are shown in Figs. 10 and 11, respectively, through profiles of liquid saturation and temperature. The temperature profiles are shown by the dashed curves while the saturation is given by the solid curves; the temperature and saturation curves intersect in the figures at the phase front. Note in Figs. 10 and 11 that the upstream weighted results give a phase front that is farther advanced relative to the LTVD result.

Unlike typical phase displacement problems which show minimal differences whether computed by upstream weighting or by higher-order schemes, the phase front locations in this problem are significantly different in the upstream and LTVD cases. The advancement of the upstream weighted phase front relative to the LTVD phase front occurs because upstream weighting produces greater smearing of the temperature front, so that saturation temperature at prevailing pressures is reached at somewhat larger distance from the injection point. The phase transition to two-phase conditions then also occurs at larger distance. In addition to the upstream and TVD-weighted simulations shown in Figs. 10 and 11, a third simulation not shown here was performed in which TVD-weighting was applied only to interface temperatures, while phase saturations were upstream-weighted. This produced results very close to those of Fig. 11, confirming that it is the numerical dispersion of the temperature front, not that of the phase front, which causes the upstream-weighted results in Fig. 10 to deviate from the more accurate LTVD results of Fig. 11.

The differences between the uptream and LTVD schemes diminish with increased resolution. We show in Fig. 12 a summary of the results of phase front location vs. number of gridblocks at a time of 6 months for this one-dimensional injection and production problem. Note in Fig. 12 that the two schemes are converging slowly but that the LTVD scheme was closer to the grid-converged result at much coarser resolution. When upstream weighting is used, numerical dispersion is proportional to ΔY (the grid spacing), and therefore diminshes slowly when grids are refined. Note finally that the fact that the saturation variation increases with time in this problem posed no problem for the LTVD scheme.

Table 3. Parameters for injection problem.

Formation	
Length	200 m
Rock grain density (ρ_R)	2650 kg m^{-3}
Specific heat (c_R)	1000 J kg^{-1} ˚C^{-1}
Thermal conductivity	2.1 W m^{-1} ˚C^{-1}
Porosity (ϕ)	0.50
Permeability	1 x 10^{-12} m^2

Relative permeability: Corey curves with $S_{lr} = 0.30$, $S_{gr} = 0.05$	
Initial temperature	300 ˚C
Initial liquid saturation	0.99
Initial pressure	85.93 bar
Production/Injection	
Production rate	0.4 kg s^{-1}
Injection rate	0.4 kg s^{-1}
Injection enthalpy	125 kJ kg^{-1}

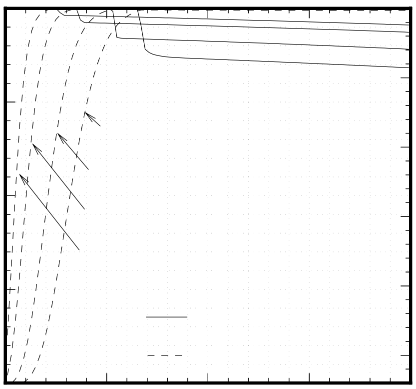

Fig. 10. Liquid saturation and temperature for the geothermal injection and production problem with upstream weighting.

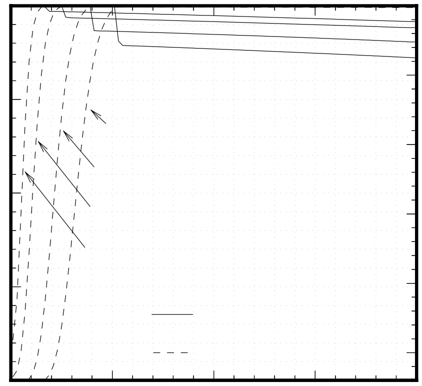

Fig. 11. Liquid saturation and temperature for the geothermal injection and production problem with LTVD.

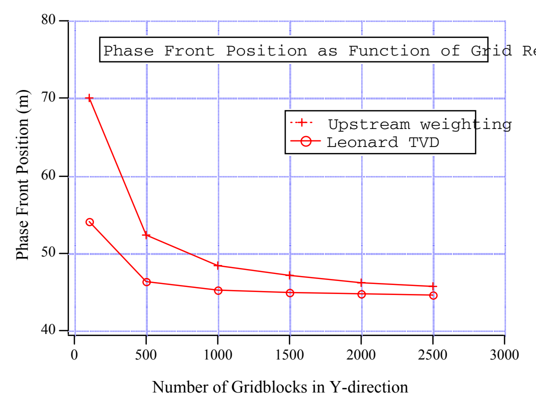

Fig. 12. Phase front location vs. grid resolution for upstream weighting and LTVD schemes at $t = 6$ mo.

CONCLUSIONS

The LTVD scheme reduces numerical dispersion of phase saturation fronts relative to upstream weighting for phase front propagation problems. However, because of self-sharpening effects, the improvement in results with LTVD relative to upstream weighting is minimal for many phase front propagation problems. In other more complicated situations where the flow is not TVD, such as the case of flow through composite porous media or under boiling conditions, LTVD reduces numerical dispersion and avoids spurious oscillations that sometimes arise in other higher-order differencing schemes. Simulations of isothermal phase front propagation in composite porous media have shown that higher-order differencing schemes should be based on saturation (S) as opposed to relative permeability (k_r). For linear relative permeability functions or for homogeneous porous media, it is immaterial whether the higher-order scheme is based on S or k_r. In geothermal injection and production problems where boiling occurs, the location of the phase front may be very sensitive to the choice of weighting scheme. Our simulations show that the LTVD scheme is more accurate for the boiling front problem at a given discretization than upstream weighting, but that resolution of temperature fronts and phase front location is sensitive to grid resolution for both schemes.

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REFERENCES

Aziz, K. and A. Settari. *Petroleum Reservoir Simulation*, Elsevier, London and New York, 1979.

Blunt, M., and B. Rubin, Implicit flux limiting schemes for petroleum reservoir simulation, *J. Comput. Physics*, *102*, 194–210, 1992.

Datta-Gupta, A., L.W. Lake, G. A. Pope, and K. Sepehnoori, High-resolution monotonic schemes for reservoir fluid flow simulation, *In Situ*, *15*(3), 289–317, 1991.

Leonard, B.P., Third-order upwinding as a rational basis for compuational fluid dynamics, in *Computational Techniques and Applications*, Elsevier Science Publishers, North-Holland, 1984.

Oldenburg, C.M. and K. Pruess, Mixing with first-order decay in variable-velocity porous media flow, *Transport in Porous Media*, *22*, 161–180, 1996.

Oldenburg, C.M. and K. Pruess, Higher-order differencing for geothermal reservoir simulation, Proc. 22nd Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford CA, January 27–29, 1997. SGP-TR-155

Pruess, K., TOUGH User's Guide, *Nuclear Regulatory Commission, Report NUREG/CR-4645*, June 1987 (also *Lawrence Berkeley Laboratory Report*, *LBL-20700*, June 1987).

Pruess, K., TOUGH2- A general-purpose numerical simulator for multiphase fluid and heat flow, *Lawrence Berkeley National Laboratory Report LBL-29400*, May 1991.

Sweby, P.K., High resolution schemes using flux limiters for hyperbolic conservation laws, *SIAM J. Numer. Anal.*, *21*(5), 995–1011, 1984.

Taggert, I.J., and W.V. Pinczewski, The use of higher order differencing techniques in reservoir simulation, *SPE Reser. Eng.*, *2*, 360, 1987.

Thomas, G.W., *Principles of Hydrocarbon Reservoir Simulation*, Intl. Human Resources Development Corporation, Boston, 1982.

Wu, Y.-S., K. Pruess, and Z.X. Chen, Buckley-Leverett flow in composite porous media, *SPE Advanced Technology Series, 1*(2), 1993.